

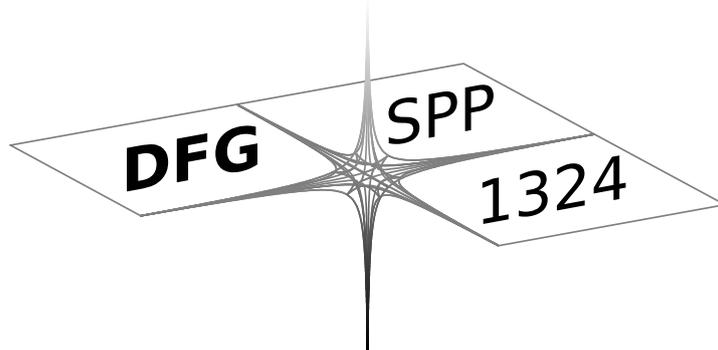
# DFG-Schwerpunktprogramm 1324

„Extraktion quantifizierbarer Information aus komplexen Systemen“

## An adaptive wavelet method for parameter identification problems in parabolic partial differential equations

S. Dahlke, U. Friedrich, P. Maass, T. Raasch, R.A. Ressel

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Philipps-Universität Marburg  
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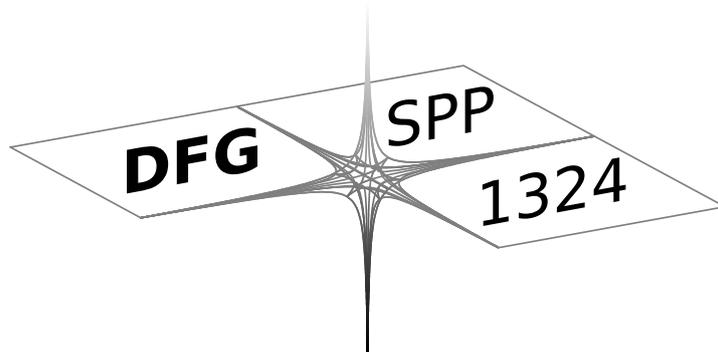
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# An Adaptive Wavelet Solver for a Nonlinear Parameter Identification Problem for a Parabolic Differential Equation

Stephan Dahlke<sup>†</sup>    Ulrich Friedrich<sup>†</sup>    Peter Maaß\*  
Thorsten Raasch<sup>‡</sup>    Rudolf A. Ressel\*

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In this paper, we combine concepts from two different mathematical research topics: Adaptive wavelet techniques for well-posed problems and regularization theory for inverse problems. We are concerned with identifying certain parameters in a parabolic reaction-diffusion equation from measured data. The PDE describes the gene concentrations in embryos at an early state of development. The forward problem is formulated as an evolution equation, and the analytical properties of the parameter-to-state operator are analyzed. The results justify the application of an iterated soft-shrinkage algorithm within a Tikhonov regularization approach. The forward problem is treated by means of a new adaptive wavelet algorithm which is based on tensor wavelets. An implementation of this procedure involving the new adaptive wavelet solver is proposed and numerical results are presented.

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\*Center for Industrial Mathematics / Fachbereich 3, University of Bremen, Postfach 33 04 40, 28334 Bremen, Germany, {[ressel](mailto:ressel@math.uni-bremen.de),[pmaass](mailto:pmaass@math.uni-bremen.de)}@math.uni-bremen.de;  
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<sup>†</sup>Philipps-University Marburg, Fachbereich 12, Hans-Meerwein-Str., 35032 Marburg, Germany, {[dahlke](mailto:dahlke@mathematik.uni-marburg.de),[friedrich](mailto:friedrich@mathematik.uni-marburg.de)}@mathematik.uni-marburg.de;  
S. Dahlke and U. Friedrich were supported by Deutsche Forschungsgemeinschaft, grant number DA 360/12-1. S. Dahlke also acknowledges support by the LOEWE Center for Synthetic Microbiology, Marburg.

<sup>‡</sup>Johannes Gutenberg-University, Institute of mathematics, Staudingerweg 9, 55099 Mainz, Germany, [raasch@uni-mainz.de](mailto:raasch@uni-mainz.de)

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## 1 Introduction

For about 30 years the advances of experimental techniques in genetic research have produced an abundance of data on gene expression in model systems. With full justification one may say that genetic research has matured enough for the application of mathematical methods permitting the extraction of structural information from this compiled data. A particularly popular object of genetic research is the *Drosophila* fly in which by genetic manipulation one may investigate the effect and the mutual interaction of certain genes on the development of the animal. However, conducting these experiments in-vitro is a challenging process. Therefore it is desirable to explore the possibilities of deducing certain critical parameters in the animal's metabolism from the measured expression of genes at certain times of its life cycle. One approach in studying gene regulation is to consider gene product concentrations as the state variables of a model and to assume that mutual gene interactions correspond to the synthesis rate of mentioned gene products [RS95].

Mathematically this amounts to solving an operator equation of the kind

$$\mathfrak{D}(p) = y,$$

where  $\mathfrak{D}$  is the so called control-to-state operator mapping the model parameters  $p$  to the data  $y$ . In the case of embryogenesis models, the set of parameters  $p$  includes reaction and diffusion coefficients and the resulting vector-valued function  $y$  denotes the concentration of different genes at different times and locations. The data is usually contaminated with noise, i.e., we have to work with  $y_{data}$ ,  $\|y - y_{data}\| \leq \delta$ . Also, it may be available only at certain points in time. The operator  $\mathfrak{D}$  is nonlinear and ill-posed, so regularization techniques have to be employed. The reader unfamiliar with regularization may consult standard references such as the monographs [Lou89] or [EHN96].

We use Tikhonov regularization to reformulate our inverse problem as finding the minimizer of the functional

$$\|\mathfrak{D}(p) - y_{data}\|^2 + \alpha J(p).$$

The choice of the penalty term gives some leeway to enforce certain characteristics of the solution. One rather popular approach is to assume the solution exhibits sparsity with respect to some appropriately chosen discretization. The biology of the underlying problem in fact justifies this hypothesis: the action taking place is localized and

the mutual influence of all genes on the synthesis of one particular gene is limited, i.e., only few genes interfere with one particular gene. For the case of an linear operator  $\mathfrak{D}$  [DDD04] provides a numerically appealing algorithm and proves convergence for the choice  $J(p) = \|p\|_{w,q}^q$ ,  $1 \leq q \leq 2$ , where the norm denotes a weighted sequence norm of the coefficients of  $p$  with respect to some Riesz basis. Several approaches for generalizing such schemes for nonlinear operator equations have been proposed recently. We will follow the iterated soft shrinkage approach which was introduced and analyzed in [BLM09]. We exemplify the use of such algorithms for a parameter identification problem induced by the nonlinear parabolic PDE (1) which serves as a basic model for the evolution of gene expressions in embryogenesis. We refer to Subsection 2.1 for a detailed explanation.

A very powerful technique for the constructive approximation of solutions to operator equations are adaptive schemes. The crucial concept of adaptivity is to update some underlying grid or function space according to some a posteriori estimator only in the regions where the local error exceeds some predetermined bound. In the context of finite element schemes, adaptive algorithms have a long and very successful history. We refer e.g. to [Ver96] for an overview. Moreover, quite recently the design of adaptive algorithms based on wavelets has lead to a fundamental breakthrough. Indeed, in [CDD01, CDD02] an adaptive algorithm that is guaranteed to converge for a huge class of problems, including operators of negative order, has been designed. Moreover, the approximation order of these algorithms is optimal in the sense that they asymptotically realize the convergence order of best  $N$ -term wavelet approximation.

So far, the whole theory is well-developed for boundedly invertible operators. Some effort has been spent to generalize these ideas also to inverse problems, we refer, e.g., to [DFR09, RTZ08], but this field is still in its infancy. However, since we utilize an iterative approach, we can take advantage of mentioned adaptive algorithms at least for the forward problem, since this is well-posed. In this paper, we use a recently developed variant of the classical wavelet algorithms, i.e., we employ an adaptive scheme based on (anisotropic) tensor wavelets. Standard (isotropic) wavelets span a complement space between consecutive spaces of a multi-resolution analysis.

On product domains which are considered here, one has the possibility to define (anisotropic) wavelet bases as the tensor product of univariate bases. Such a tensor basis contains the so-called sparse grids or hyperbolic cross spaces [BG04, Zen91]. It is known that a function with  $L_2$  bounded mixed derivatives of a sufficiently large order can be approximated from sparse grid spaces at a rate that does not deteriorate as a function of the space dimension (the so-called curse of dimensionality is avoided). As demonstrated in [DSS09, SS08] also in the tensor product setting, adaptive wavelet methods realize the rate of best  $N$ -term approximation in linear complexity. Therefore, adaptive tensor wavelet algorithms are very suitable for the problems we are concerned with here.

Iterated soft shrinkage requires the solution of a forward problem and some adjoint equation given by their expansion in some Riesz basis. Precisely for this purpose the adaptive wavelet strategy is ideally suited. It computes solutions in their coefficient representation. Furthermore it can take full advantage of the solutions sparsity because

of its optimality.

In summary we are faced with the following problems: First of all one needs to identify the spaces between which  $\mathfrak{D}$  acts, so that the regularization becomes feasible. Then the operator  $\mathfrak{D}$  and its analytical behavior require some investigation. A third major issue is the right choice of the penalty term  $J$  that depends on the nature of the problem. Moreover, as an important building block, an efficient solver for the forward problem has to be designed.

Therefore the outline of the paper looks as follows. In Section 2 we describe the biological model problem which we choose to represent by the nonlinear parabolic equation (1). The next step is the investigation of the parameter and solution spaces. It turns out that our choice of such spaces makes the elliptic part of our differential operator continuously differentiable with respect to the parameters. Then we take a closer look at the nonlinear right-hand side of our PDE: We prove continuity and differentiability for our setting. Furthermore, we establish some local kind of Hölder continuity for the nonlinear right-hand side operator. Then the existence and uniqueness of a solution to (1) is shown, employing the results of [Grö89] and [Grö92]. In Section 3 we analyse the mapping properties of the control-to-state map  $\mathfrak{D}$ . By means of the implicit function theorem we establish its differentiability. Further analysis of the derivative shows it is even locally Hölder continuous for our choice of the parameter space. The adjoint is identified which is needed later in the regularization scheme. In Section 4 a regularization procedure is derived. We state (our adaption of) the generalized conditional gradient method and its numerical implementation as a soft-shrinkage procedure.

After having proposed the general regularization procedure, we are concerned with the adaptive numerical solution of the forward problem. In Section 5 we explain the basic ideas of adaptive wavelet algorithms with a special emphasis on the tensor wavelet setting and on elliptic equations. Moreover, we describe how adaptive strategies can be used to treat also parabolic equations. Our approach is based on the Rothe method, i.e., the parabolic equation is first discretized in time and then in space. For stability reasons, one has to use an implicit scheme, so that an elliptic subproblem has to be solved in each time step. To this end, the adaptive tensor wavelet algorithms are employed. Finally in Section 6 numerical results for the overall scheme applied to a test problem in 2 dimensions are presented.

## 2 Analysis of the forward problem

In this section, we state and analyse the forward problem as far as it is needed for our purposes. First of all, we state and discuss the biological model we will be concerned with. Then, in Subsection 2.2, we provide all the necessary building blocks such as suitable function spaces and nonlinear operators. Finally, in Subsection 2.3, we prove the existence and uniqueness of a solution of (1).

## 2.1 The biological model

The state variables, the concentrations of gene products, undergo permanent change over time. One of the assumed reasons this change is direct regulation of the synthesis of one gene by the concentrations of other genes; further causes are diffusive processes of gene products through the admissible domain and decay, i.e., consumption, of the respective gene products. The synthesis requires some regulating function in a manner that reflects saturation in the signal response.

A mathematical formulation is given as follows. Let  $U$  denote some open Lipschitz domain contained in  $\mathbb{R}^n$ ,  $n = 2, 3$ , and  $U_T = U \times (0, T]$ . The concentration of the  $i$ -th gene on this space-time domain is denoted by  $g_i$ . Then the gene expression evolution is modeled by the reaction-diffusion equation

$$\begin{aligned} \frac{\partial g_i}{\partial t} - \operatorname{div}(D_i(x, t)\operatorname{grad}g_i(x, t)) + \lambda_i(x, t) \cdot g_i(x, t) &= R_i(x, t)\Phi_i((W(x, t)g(x, t))_i), \quad (x, t) \in U_T \\ \frac{\partial g_i}{\partial \nu} &= 0 \quad (x, t) \in \partial U \times [0, T], \quad g(0) = g_0 \quad \text{on } U \times \{0\} \end{aligned} \quad (1)$$

where  $i = 1, \dots, N$ , and the function

$$\Phi_i : \mathbb{R} \rightarrow \mathbb{R}; \quad \Phi_i(y) = \frac{1}{2} \left( \frac{y}{\sqrt{y^2 + 1}} + 1 \right) \quad (2)$$

is a sigmoidal response function. For the right-hand side we assume  $g_0 \in W_2^1(U, \mathbb{R}^N)$  and the parameters are to be contained in certain  $L_p$  spaces

$$\begin{aligned} D &\in L_{p_D}(U \times [0, T], \mathbb{R}^N), & \lambda &\in L_{p_\lambda}(U \times [0, T], \mathbb{R}^N), \\ R &\in L_{p_R}(U \times [0, T], \mathbb{R}^N), & W &\in L_{p_W}(U \times [0, T], \mathbb{R}^{N \times N}). \end{aligned} \quad (3)$$

The exponent  $p_D$  we choose as  $p_D = \infty$ . The exponents  $2 \leq p_\lambda, p_R, p_W < \infty$  will be specified later on. The particular choice of these parameters must guarantee the existence and uniqueness of solutions for our PDE in some appropriate solution space.

The diffusion term with the spatially and temporally varying diffusion parameter  $D$  accounts for the transport of gene products. A linear decay term is modelled by the parameter  $\lambda$ . Finally and most interestingly is a synthesis term  $R\Phi(Wg)$  with a maximal synthesis rate  $R$  multiplied with some signal response (or regulation-expression) function. This signal response function takes as the input arguments the concentrations of all the gene products present. Our particular choice of this signal response function, which is justified in the fundamental paper [MSR91], is a sigmoidal  $\Phi$  applied to each component of the product of some parametric interaction matrix  $W$  and the array of gene products  $g$ . Notice that negative entries in  $W$  correspond to an inhibiting influence of one gene product on the other and positive ones represent an amplifying effect.

One important aspect in the choice for the topology of the parameter space are the requirements of regularization. We choose certain subspaces of Bochner integrable functions (i.e., generalized Sobolev spaces) as the solution spaces. The most straightforward and common choice for the admissible set of parameters  $\lambda$ ,  $R$ , and  $W$  might be subsets

of  $L_\infty$  spaces. However, we want to apply generalized gradient methods which involve the dual space of the parameter space. The  $L_\infty$  topology would then require dealing with the very inconvenient dual of some  $L_\infty$  product space. Whenever theory permits, we will try to avoid this. We therefore choose as our parameter sets all functions in  $L_\infty$  fulfilling the bounds

$$0 < C_{\mathcal{P},1} \leq D, \lambda \leq C_{\mathcal{P},2}, \quad 0 \leq R \leq C_{\mathcal{P},2}, \quad \|W\|_\infty \leq C_{\mathcal{P},2},$$

endowed with particular  $L_p$  norms as indicated above. The parameter space for  $D$  is  $\mathcal{P}_D = \{D \in L_{p_D} : 0 < C_{\mathcal{P},1} \leq D \leq C_{\mathcal{P},2}\}$ . Accordingly, we define the parameter spaces  $\mathcal{P}_\lambda, \mathcal{P}_R, \mathcal{P}_W$ . The global parameter space we denote as

$$\mathcal{P} = \mathcal{P}_D \times \mathcal{P}_\lambda \times \mathcal{P}_R \times \mathcal{P}_W \quad (4)$$

equipped with the usual product norm of the individual spaces. Observe that by the finiteness of  $U$ , the boundedness conditions of the individual parameters imply that the parameter space is contained in a subset bounded in the norm of  $\mathcal{P}$ .

Another aspect will affect our choice of the exponents  $p_R, p_\lambda, p_W$ . Namely, we need to ensure the PDE solutions depend differentiably on the parameters.

## 2.2 Function spaces, operators

### 2.2.1 The solution space

We will develop the solution theory for the well-known spaces of Bochner integrable functions. The general definitions and basic theory about these spaces can be found in [Sho97, ChIII.1-2].

Let us now fix the notation for our setting. We introduce the spaces

$$\begin{aligned} V_q &= W_q^1(U, \mathbb{R}^N), \\ \mathcal{V}_s &= L_s(0, T; V_q) \end{aligned}$$

with  $q \in (n, n + \epsilon)$  where  $\epsilon > 0$  will be specified later on and  $s \in (1, \infty)$ . The conjugate exponent we will denote by  $q'$ , i.e.  $1/q + 1/q' = 1$ . When we consider derivatives of elements from  $\mathcal{V}_q$ , e.g.  $u'$ , these will be distributional derivatives. With these conventions we define the generalized Sobolev space

$$\mathcal{W}_s = \{u \in L_s(0, T; V_q) : u' \in L_s(0, T; V_{q'})\}, \quad \|u\|_{\mathcal{W}_s} = \|u\|_{L_q(0, T; V_q)} + \|u'\|_{L_s(0, T; V_{q'})}.$$

A particular kind of this type of space we will use as the solution space later on.

In order to show differentiability of the nonlinear right-hand side in our PDE we need to be able to embed  $\mathcal{W}_s$  into a spaces with higher integrability.

**Theorem 1.** Let  $q > n$ . Then there is a continuous embedding  $\mathcal{W}_s \hookrightarrow L_r(0, T; L_r(U, \mathbb{R}^N))$ , where  $r$  can be chosen from  $r \in (q, \infty)$ .

*Proof.* The proof can be found in [Res11, Ch. 2.2.2]. □

Now we shall put  $q = \mathfrak{q}$ , such that  $q \in (n, n + \epsilon)$  and  $\epsilon = \epsilon(U, C_{\mathcal{P},1}, C_{\mathcal{P},2}) > 0$  is as in [HDR09, Thm. 5.14]. This choice then ensures the solvability of our PDE as according to the findings of [HDR09] (see Section 2.3). Furthermore we let  $s = \mathfrak{q}$ . This choice of  $s$  is mainly to ease notation. Interested readers can easily generalize all the results below for another choice of  $s \in (1, \infty)$  (according to the requirements of [HDR09]) by introducing a second array of exponents of integrability for the time domain.

We fix a particular  $\mathfrak{r} > \mathfrak{q}$  and define

$$\mathcal{W} = \mathscr{W}_{\mathfrak{q}} = \{u \in \mathcal{V}_{\mathfrak{q}} : u \in (\mathcal{V}_{\mathfrak{q}'})'\} \quad \text{where} \quad \|u\|_{\mathcal{W}} = \|u\|_{\mathcal{V}_{\mathfrak{q}}} + \|u'\|_{(\mathcal{V}_{\mathfrak{q}'})'}. \quad (5)$$

The space  $\mathcal{W}$  will serve as the solution space for (1), see Section 2.3.

We specify  $p_{\lambda}$  in the following fashion:

$$\frac{1}{p_{\lambda}} + \frac{1}{\mathfrak{r}} \leq \frac{1}{\mathfrak{q}}. \quad (6)$$

This condition on  $p_{\lambda}$  guarantees that the elliptic operator in (1) fulfills the smoothness conditions needed later. The elliptic part of our model PDE (1) defines the bilinear operator

$$\begin{aligned} \mathcal{A} : \mathcal{P} \times \mathcal{W} &\rightarrow \mathcal{V}'_{\mathfrak{q}'}, \\ \mathcal{A}(p, u)(\phi) &= \int_0^T \int_U \langle D(x, t) \nabla u(x, t), \nabla \phi(x, t) \rangle + \lambda(x, t) u(x, t) \phi(x, t) \, dx. \end{aligned} \quad (7)$$

In the following statement the operator  $\frac{d}{dt} : \mathcal{W} \rightarrow \mathcal{V}'_{\mathfrak{q}'}$ ,  $u \mapsto u'$  is to be understood as the distributional derivative operator. Then

**Theorem 2.** The differential operator  $\frac{d}{dt} + \mathcal{A} : \mathcal{P} \times \mathcal{W} \rightarrow \mathcal{V}'_{\mathfrak{q}'}$  is well-defined and continuous.

We obtain for the differential operator (bounded) continuity and therefore continuous differentiability with respect to both input arguments  $u$  and  $(D, \lambda)$ .

### 2.2.2 Nonlinear Operators

To handle the nonlinear right-hand side of our PDE (1) we need to introduce some concepts. For a comprehensive treatment of these nonlinearities, so-called superposition operators, the reader may consult the standard reference [AZ90]. As an aside we mention that the proofs in the following theorems rely chiefly on the particular choice of the exponents  $p_R$  and  $p_W$ , which shall be

$$\frac{1}{p_R} + \frac{1}{p_W} + \frac{1}{\mathfrak{r}} \leq \frac{1}{\mathfrak{q}}. \quad (8)$$

Another important ingredient will be analytic qualities of the signal response function. Namely the smoothness, global Lipschitz continuity and global boundedness of  $\Phi : \mathbb{R} \rightarrow \mathbb{R}$  and its derivatives matter and therefore  $\Phi$  can be replaced by another signal response function as long as the replacement suffices these conditions as well.

By the results in [AZ90] we obtain

**Lemma 3.** Let  $W \in \mathcal{P}_W, R \in \mathcal{P}_R$ , and the signal response function  $\Phi$  given by (2). Then the map

$$\begin{aligned} F : L_{\mathfrak{r}}(0, T; L_{\mathfrak{r}}(U, \mathbb{R}^N)) &\rightarrow L_{\mathfrak{q}}(0, T; L_{\mathfrak{q}}(U, \mathbb{R}^N)), \\ u \mapsto (F_i(u))_{i=1}^N &= (R_i(x, t)\Phi((W(x, t)u(x, t))_i))_{i=1}^N \end{aligned} \quad (9)$$

is continuous.

Concerning the differentiability of a nonlinear operator such as the above we infer from [AZ90, Thm 3.13] that

**Theorem 4.** The operator  $F$  as defined in Equation (9) is continuously differentiable. Fixing  $\mathfrak{p} = \frac{\mathfrak{q}\mathfrak{r}}{\mathfrak{r}-\mathfrak{q}}$  the derivative is given by

$$\begin{aligned} F' : L_{\mathfrak{r}}(0, T; L_{\mathfrak{r}}(U, \mathbb{R}^N)) &\rightarrow L_{\mathfrak{p}}(0, T; L_{\mathfrak{p}}(U, \mathbb{R}^N)), \\ u \mapsto (F'_i(u))_{i=1}^N &= (R_i(x, t)\Phi'((W(x, t)u(x, t))_i)W_i(x, t))_{i=1}^N. \end{aligned} \quad (10)$$

$F'$  is locally Hölder continuous.

As a simple consequence of [AZ90, p. 105] we also obtain

**Theorem 5.** For  $\mathfrak{r}, p_W$  and  $p_R$  as above the operator defined in (10) is Hölder continuous on bounded sets with Hölder exponent  $\gamma = 1/\mathfrak{b}$ , where  $\mathfrak{b} = (1/p_W + 1/\mathfrak{r})^{-1}$ .

When fixing the function  $u$  and varying the parameters  $R$  and  $W$  instead in their admissible range, we obtain analogous statements for the continuous differentiability of the right-hand side operator viewed as a function of  $R$  and  $W$ .

## 2.3 Solvability

A weak formulation of our model PDE can be stated as follows.

**Definition 6.** A function  $u \in \mathcal{V}_{\mathfrak{q}}$  is a weak solution of the PDE (1), iff

$$u \in \mathcal{W} : \quad u' + \mathcal{A}u = F(u) \quad \text{in} \quad \mathcal{V}'_{\mathfrak{q}'}, \quad u(0) = u_0 \in G, \quad (11)$$

where  $\mathcal{A}$  and  $F$  are defined in (7) and (9), respectively.  $G$  is defined as the trace space  $G = (V_{\mathfrak{q}}, (W_{\mathfrak{q}'}^1)')_{(1/\mathfrak{q}', \mathfrak{q})} = B_{\mathfrak{q}, \mathfrak{q}}^m(U, \mathbb{R}^d)$ , with  $m = 1 - 2/\mathfrak{q}$  and the last identity follows from standard results about Besov spaces (see [Tri95, 2.4.2 Rem 2b), 4.3.1 Thm. 2]).

The main result of this subsection then reads as follows.

**Theorem 7.** The Cauchy problem as stated in equation 11 has a unique solution.

**Remark 8.** For the readers convenience let us briefly sketch the ideas of the proof. We consider the linearized problem

$$u \in \mathcal{W} : \quad u' + \mathcal{A}u = f \quad \text{in } \mathcal{V}'_q, \quad u(0) = u_0 \in G, \quad (12)$$

where the right-hand side is obtained by  $f(t) = F(t, w(t)) \in \mathcal{V}'_q$  for some arbitrary  $w \in C(0, T; G)$ . Then the results of [Res11, Ch. 2.3] building on the main statements in [HDR09, ACFP07] imply that (12) has a unique solution that depends continuously on  $f$ .

Let  $B : C(0, T; G) \rightarrow C(0, T; G)$  be the map which assigns to  $w$  the unique solution of (12) with right-hand side  $f = F(w)$  (note that there exists a continuous embedding  $\mathcal{W} \hookrightarrow C(0, T; G)$ ). Then an application of Banach's fixed point theorem yields the result.

## 3 The control-to-state map

### 3.1 Continuity and differentiability of the control-to-state map

Using the setting of Section 2 we will employ the implicit function theorem to prove the desired qualities of the control-to-state operator which maps the parameters of (1) to its solution. Proofs for all the statements in this chapter can be found in the respective section on the control-to-state map in [Res11]. Therefore we have only sketched or altogether omitted the proofs here to expedite the reader's journey through the theory towards a comprehensive overview of our project. When necessary one can always confer the given reference [Res11] for proofs and further details.

In this section we consider the parameter domain  $\mathcal{P}$  as defined in (4), with the conditions on the parameters given by Equations (6),(8).

Then we introduce the operator

$$\begin{aligned} \mathfrak{C} : \quad \mathcal{P} \times \mathcal{W} &\rightarrow G \times \mathcal{V}'_q, \\ (p, u) &\mapsto (u(0) - u_0, u' + \mathcal{A}u - F(u)). \end{aligned} \quad (13)$$

Clearly this operator is well-defined: the first component is well-defined by the standard Sobolev embedding  $\mathcal{W} \hookrightarrow C([0, T]; G)$  (see [ACFP07]), and the second component is well-defined by the assumptions on  $u, \mathcal{A}$ , and  $F$ . Equipping the space  $\mathcal{P} \times \mathcal{W}$  with a product norm, we obtain a normed space. Clearly, the image space  $G \times \mathcal{V}'_q$  is also normed.

For the next lemma we fix the first argument and show continuous differentiability with respect to the second argument.

**Lemma 9.** The map  $\mathfrak{S} = \mathfrak{C}(p_0, \cdot) : \mathcal{W} \rightarrow G \times \mathcal{V}'_q$  is continuously differentiable and the derivative at any  $u$  is an isomorphism from  $\mathcal{W}$  onto  $G \times \mathcal{V}'_q$ .

*Proof.* The proof utilizes the differentiability that was proved in Theorem 4 for the nonlinear part. For the linear part of the differential operator, continuous linearity

imply continuous differentiability. The continuity of the inverse of the derivative follows from standard PDE theory. For details confer [Res11].  $\square$

By using similar arguments, one can also establish differentiability with respect to the first argument.

**Lemma 10.** The map  $\mathfrak{P} = \mathfrak{C}(\cdot, u) : \mathcal{P} \rightarrow G \times \mathcal{V}'_q$  is continuously differentiable.

*Proof.* The proof is analogous to the part of the above proof which concerns differentiability. For details confer [Res11].  $\square$

For certain non-Banach situations a modified implicit function theorem holds under stronger assumptions (see [Res11]). Fortunately, such an assumption holds for our case so we can use this modified version of the implicit function theorem together with the last two lemmata to make the following statement:

**Corollary 11.** The control to state map  $\mathfrak{D} : \mathcal{P} \rightarrow \mathcal{W}$ ,  $p \mapsto u$ , assigning to each tuplet of parameters  $p$  the unique solution of (11), is continuously differentiable. We obtain a formula for the derivative of the control to state map  $\mathfrak{D}$ . Let  $v$  denote the solution to the Cauchy problem

$$v' + \mathcal{A}_0 v - R_0 \Phi'(W_0 u) W_0 v = -\mathcal{A}_1 u + R_1 \Phi(W_0 u) + R_0 \Phi'(W_0 u) W_1 u, \quad v(0) = 0$$

where  $u = u(p_0) = \mathfrak{D}(p_0)$ , then

$$\mathfrak{D}'(p_0)(p_1) = -\left(\frac{\partial \mathfrak{C}}{\partial u}\right)^{-1}(p_0, u) \circ \frac{\partial \mathfrak{C}}{\partial p}(p_0, u)(p_1) = v.$$

### 3.2 Properties of the derivative of the control to state map

The last result, namely the explicit formula for the derivative of the control to state map at some  $p_0$ , enables us to investigate further useful properties of  $\mathfrak{D}'$ . Our inspection will be divided into several lemmata, which then allow us to show Lipschitz continuity for operator  $\mathfrak{D}$  and Hölder continuity for  $\mathfrak{D}'$  on bounded sets.

**Lemma 12.** The map  $\mathfrak{D}'(\cdot) : \mathcal{P} \rightarrow \mathcal{L}(\mathcal{P}, \mathcal{W})$  is bounded on bounded sets.

*Proof.* The proof relies on the usual stability estimates for solutions of parabolic PDE and the pointwise boundedness of the parameters. For details confer [Res11].  $\square$

By applying the mean value theorem (compare [Wer00, Satz III.5.4b]) to  $\mathfrak{D}$  we obtain

**Lemma 13.** The map  $\mathfrak{D} : \mathcal{P} \rightarrow \mathcal{W}$  is Lipschitz continuous on convex, bounded sets.

*Proof.* Choose some  $\theta > 0$ . By the mean value theorem we have for  $p_0, p_1 \in \mathcal{P}$ , and  $M = \{\tilde{p} \in \mathcal{P} : \tilde{p} = \theta p_0 + (1 - \theta)p_1, \theta \in (0, 1)\}$

$$\|\mathfrak{D}(p_0) - \mathfrak{D}(p_1)\|_{\mathcal{W}} \leq \sup_{\tilde{p} \in M} (\|\mathfrak{D}'(\tilde{p})\|_{\mathcal{L}(\mathcal{P}, \mathcal{W})} \|p_0 - p_1\|_{\mathcal{P}}),$$

and the supremum in the estimate exists by the preceding lemma.  $\square$

**Lemma 14.** The operator

$$\begin{aligned} \frac{\partial \mathfrak{C}}{\partial u} : \mathcal{P} \times \mathcal{W} &\rightarrow \mathcal{L}(\mathcal{W}, G \times \mathcal{V}'_q), \\ (p_0, u) &\mapsto (h \mapsto (h(0), h' + \mathcal{A}_0 h - R_0 \Phi'(W_0 u) W_0 h)), \end{aligned}$$

is locally Hölder continuous with Hölder constant depending on  $\Phi'$  and the bound of the local set. The Hölder exponent is  $\gamma$  (as in Thm. 5).

*Proof.* The proof rests essentially on the Hölder continuity which was proved for the nonlinearity in Theorem 5. For a detailed presentation confer [Res11].  $\square$

Using a theorem concerning the differentiability of operator inversion (see [Ber74, Cor 50.3]), we can deduce the following

**Corollary 15.** The map

$$\begin{aligned} \left(\frac{\partial \mathfrak{C}}{\partial u}\right)^{-1}(\cdot, \cdot) : \mathcal{P} \times \mathcal{W} &\rightarrow \mathcal{L}(G \times \mathcal{V}'_q, \mathcal{W}) \\ (p_0, u) &\mapsto ((v_0, f) \mapsto \text{solution of } h' + \mathcal{A}_0 h - R_0 \Phi'(W_0 u) W_0 h = f, h(0) = v_0) \end{aligned}$$

is locally Hölder continuous.

**Lemma 16.** The operator

$$\begin{aligned} \frac{\partial \mathfrak{C}}{\partial p} : \mathcal{P} \times \mathcal{W} &\rightarrow \mathcal{L}(\mathcal{P}, G \times \mathcal{V}'_q) \\ (p_0, u) &\mapsto (p_1 \mapsto (0, \lambda_1 u - \text{div}(D_1 \nabla u) - R_1 \Phi(W_0 u) - R_0 \Phi'(W_0 u) W_1 u)) \end{aligned}$$

is locally Hölder continuous with Hölder constant depending on the bound of the considered set and  $\Phi'$ .

*Proof.* Similarly to the proof the preceding lemma concerning concerning  $\frac{\partial \mathfrak{C}}{\partial p}$ , the proof can be played back to the Hölder continuity of the nonlinearity. For details confer [Res11].  $\square$

An elementary statement is the following

**Lemma 17.** Let  $X_1, X_2$  be subsets of possibly different Banach spaces and  $Y$  a Banach space. Given some Hölder continuous  $f : X_1 \times X_2 \rightarrow Y$  and some Lipschitz continuous  $g : X_1 \rightarrow X_2$ , the composition  $h : X_1 \rightarrow X_2, h(x) = f(x, g(x))$  is Hölder continuous (with the same Hölder exponent as for  $f$ ).

*Proof.* Straightforward.  $\square$

The following theorem is an application of Lemmata 16,17 and Corollary 15.

**Theorem 18.** The map  $\mathfrak{D}'$  is locally Hölder continuous.

In order to apply a gradient descent scheme in Tikhonov regularization, we need to identify the derivative of the discrepancy

$$\|\mathfrak{D}(p) - y_{data}\|_{\mathcal{G}}^2,$$

where  $\mathfrak{D}(p)$  is naturally embedded via  $Inc : \mathcal{W} \rightarrow \mathcal{G} = L_2(0, T; L_2(U, \mathbb{R}^d))$ . The remaining major task in this is to compute the action of the adjoint operator of  $\mathfrak{D}'$ . One derives

$$(\mathfrak{D}'(p_0))^* = - \left( \frac{\partial \mathfrak{C}}{\partial p}(p_0, u) \right)^* \circ \left( \left( \frac{\partial \mathfrak{C}}{\partial u} \right)^{-1}(p_0, u) \right)^*. \quad (14)$$

**Remark 19.** For later use the formula of the operator  $(\mathfrak{D}'(p_0))^*$  will be given explicitly. Concerning the inner part  $\left( \frac{\partial \mathfrak{C}}{\partial u} \right)^{-1}(p_0, u)^*$  let  $\mathcal{K}$  be defined by

$$\begin{aligned} \mathcal{K} : \mathcal{P} \times \mathcal{W} &\rightarrow \mathcal{V}'_{q'}, \\ v &\mapsto \mathcal{A}v - R_0 \Phi'(W_0 u) W_0 v, \end{aligned} \quad (15)$$

with  $\mathcal{A}$  given by (7). Then a straightforward computation shows that  $\left( \frac{\partial \mathfrak{C}}{\partial u} \right)^{-1}(p_0, u)^*$  maps  $w \in \mathcal{G}$  to the solution of the PDE problem

$$-v' + \mathcal{K}v = w \text{ in } \mathcal{V}'_{q'}, \quad v(T) = 0. \quad (16)$$

Similarly the adjoint of the outer operator  $\left( \frac{\partial \mathfrak{C}}{\partial p} \right)(p_0, u) : \mathcal{P} \rightarrow G \times \mathcal{V}'_q$  is given by

$$\tilde{g} = (g_0, g) \mapsto (\langle \nabla g_i, \nabla u_i \rangle, g_i u_i, -g_i \cdot \Phi((W_0 u)_i), -g_i \cdot R_{0,i} \Phi'((W_0 u)_i) u^T)_{i=1}^N. \quad (17)$$

## 4 Regularization

### 4.1 The generalized conditional gradient method

After the examination of the forward operator we choose Tikhonov regularization to solve the inverse problem. Concerning the feasibility, we equip  $\mathcal{P}$  for a moment with the weak\*  $L_\infty$  topology. The weak\* continuity for the parameter-to-state operator is evident since  $L_\infty$  embeds continuously into any  $L_p$  space. We introduce an abstract penalty term  $J$ , which we assume to be weak\* lower semicontinuous and to have weak\* precompact sub-level sets. The only major issue, the closedness of the respective map of the inverse problem, can be obtained through the use of a compact embedding statement for our space  $W(0, T)$  analogously to the usual Sobolev embedding theorem. With these conventions the feasibility of Tikhonov regularization follows in the standard fashion (consult standard textbooks on inverse problems, eg [Lou89] or [EHN96]).

After one has established the feasibility of Tikhonov regularization, we now turn to the major practical problem of computing a solution  $v$  for the problem

$$v = \operatorname{argmin}_{p \in \mathcal{P}} \|\mathfrak{D}(p) - y_{data}\|_{L_2(0, T, L_2(U, \mathbb{R}^d))}^2 + \alpha J(p), \quad (18)$$

where  $\alpha$  is the regularization parameter.

A well-established procedure for solving this task in the linear case appears in the celebrated paper by [DDD04]. Its generalizations to the nonlinear case appears in [BLM09, BBLM07] for Hilbert spaces and in a different formulation also in [RT06]. However, we are dealing with Banach space topology rather than Hilbert space topology. Therefore in order to transport the statements in [BLM09] to our setting, the scalar products therein have to be read as dual pairings.

To be precise, for our setting we deal with a subset of a Banach space  $X$  and two functions  $\mathcal{E}, \mathcal{F} : X \rightarrow \mathbb{R}_0^+ \cup \infty$ . In addition to the usual norm topology on  $X$  we introduce some topology  $\tau$  on  $X$ , for which norm bounded sets are  $\tau$  compact.

The reader is cautioned not to confuse  $\mathcal{E}$  and  $\mathcal{F}$  with the terms appearing in the Tikhonov functional (eqn. 18). The connection between  $\mathcal{E}$  and  $\mathcal{F}$  and the Tikhonov functional will be given after the introduction of the algorithm presented now.

We want the following conditions to hold.

**Conditions 20.** For  $\mathcal{F}$  we assume continuous differentiability.  $\mathcal{E}$  does not need to be differentiable, but needs to satisfy

1.  $\mathcal{E}(x) < \infty$  for some  $x \in X$ .
2.  $\mathcal{E}$  is convex.
3.  $\mathcal{E}$  is sequentially  $\tau$  lower semicontinuous, ie  $\mathcal{E}(x) \leq \liminf_n \mathcal{E}(x_n)$ , whenever  $x = \lim_n x_n$ .
4.  $\mathcal{E}$  is coercive, i.e.,  $\mathcal{E}(x_n) \rightarrow \infty$ , whenever  $\|x_n\| \rightarrow \infty$ .
5. The problem  $\operatorname{argmin}_{v \in X} \mathcal{F}'(x)(v) + \mathcal{E}(v)$  has some solution.
6.  $\mathcal{E}$  has weakly compact sublevel sets.

Our intermediate target is then to solve

$$\operatorname{argmin}_{v \in X} \mathcal{F}(v) + \mathcal{E}(v). \quad (19)$$

In this setting most statements in [BLM09] remain valid. Only two aspects in this approach demand closer attention. The first is the compactness requirement on the sublevel sets of the penalty term  $\mathcal{E}$ . Since however we intend to use some weighted- $\ell_q$  penalty term,  $1 \leq q < 2$ , for  $\mathcal{E}$ , we have the freedom to impose such weights which ensure the mentioned compactness requirements. The second aspect concerns uniform continuity of the derivative of  $\mathcal{F}$ , which can be covered by the analysis of the parameter-to-state operator.

Solving our intermediate problem (19) is then handled by the GCGM algorithm:

#### ALGORITHM 21. GCGM

1. Choose  $x_0 \in X$ , such that  $\mathcal{E}(x_0) < \infty$

2. Determine  $v_n \in X$  by

$$v_n = \operatorname{argmin}_{v \in X} (\mathcal{F}'(x_n), v) + \mathcal{E}(v).$$

3. Determine stepsize  $s_n \in [0, 1]$  via

$$s_n = \operatorname{argmin}_{s \in [0, 1]} \mathcal{F}(x_n + s(v_n - x_n)) + \mathcal{E}(x_n + s(v_n - x_n)).$$

4. Put  $x_{n+1} = x_n + s_n(v_n - x_n)$ . Return to step 2.

## 4.2 Connection to iterated soft-shrinkage

In this subsection we consider the case where  $\mathcal{P}$  is a product of  $L_2$  spaces. We further assume that a (biorthogonal) Riesz-Basis ( $\Psi = \{\psi_\lambda : \lambda \in \mathcal{J}\}$ ,  $\tilde{\Psi} = \{\tilde{\psi}_\lambda : \lambda \in \mathcal{J}\}$ ) for (a subspace of)  $\mathcal{P}$  is available. The connection between the minimization Problem (18) induced by Tikhonov regularization and the proposed **GCGM** 21 becomes clear when we look at their formulation for this setting (compare also [BLM09, pp.185]). We define

$$\mathcal{F}(p) := \frac{1}{2} \|\mathfrak{D}(p) - y_{data}\|_{\mathcal{G}}^2 - \frac{1}{2} \|p\|_{\mathcal{G}}^2, \quad (20)$$

and

$$\mathcal{E}(p) := \frac{1}{2} \|p\|_{\mathcal{G}}^2 + \alpha \sum_{\lambda \in \mathcal{J}} w_\lambda |\langle p, \tilde{\psi}_\lambda \rangle|^q,$$

remarking that Conditions 20 are fulfilled. The minimization problem of eqn. 18 is then given by

$$\min_{p \in \mathcal{P}} \frac{1}{2} \|\mathfrak{D}(p) - y_{data}\|_{\mathcal{G}}^2 + \alpha \sum_{\lambda \in \mathcal{J}} w_\lambda |\langle p, \tilde{\psi}_\lambda \rangle|^q. \quad (21)$$

The following equivalent formulation of the second step of the **GCGM** is the minimization problem (applying our previous computation of  $(\mathfrak{D}'(p))^*$ ):

$$v = \operatorname{argmin}_{\rho \in \mathcal{P}} \sum_{\lambda \in \mathcal{J}} \frac{1}{2} |\langle (\mathfrak{D}'(p))^* (\mathfrak{D}(p) - y_{data}) - \rho + \rho, \tilde{\psi}_\lambda \rangle|^2 + \alpha w_\lambda |\langle \rho, \tilde{\psi}_\lambda \rangle|^q. \quad (22)$$

Given the admissible minimizer lies in the interior of  $\mathcal{P}$  the admissible set, one can derive the coefficientwise first order necessary condition which reads as :

$$\langle v, \tilde{\psi}_\lambda \rangle_{\lambda \in \mathcal{J}} = \mathbf{S}_{\alpha w, p}(\langle (p - (\mathfrak{D}'(p))^* (\mathfrak{D}(p) - y_{data})), \tilde{\psi}_\lambda \rangle_{\lambda \in \mathcal{J}}), \quad (23)$$

where  $\mathbf{S}_{\alpha w, p}$  is a shrinkage operator that applies to each coefficient the shrinkage map  $S_{\alpha w, p}$ . This map is defined by

$$S_{\alpha w, p}(c) = \begin{cases} \operatorname{sgn}(c_\lambda) [|c_\lambda| - \alpha w_\lambda]_+ & p = 1 \\ G_{\alpha w_\lambda, p}^{-1}(c_\lambda) & p > 1, \end{cases} \quad (24)$$

where  $G_{\alpha w_\lambda p}(x) = x + \alpha w_\lambda p \operatorname{sgn}(x)|x|^{p-1}$ . Precisely this coefficientwise computation makes the shrinkage algorithm numerically attractive.

In case however the minimizer is not in the interior of the admissible set, it still needs to be checked whether some projection can be employed to find the admissible minimizer on the boundary of the admissible set. In any case, after each application of the shrinkage map admissibility needs to be verified.

## 5 Discretisation of the model PDE

In this section, we briefly explain how to apply adaptive wavelet methods for the numerical solution of the model PDE (11). First of all, in Subsection 5.1, we recall the wavelet setting. Then, in Subsection 5.2, we discuss adaptive wavelet schemes for elliptic problems. Finally, in Subsection 5.3, we are concerned with generalizations to parabolic equations.

### 5.1 Wavelets

Let us briefly recall the wavelet setting as far as it is needed for our purposes. We will not go into construction details and confine the discussion to the basic facts. For the anisotropic tensor wavelet construction in arbitrary dimensions we follow [?].

We assume an univariate wavelet collection  $\Psi = \{\psi_\lambda : \lambda \in \mathcal{J}\} \subset W_2^t(\mathcal{I})$  on the unit interval  $\mathcal{I} := (0, 1)$  is available. The indices  $\lambda \in \mathcal{J}$  encode several types of information, namely the *scale* (often denoted  $|\lambda|$ ), the spatial location and also the type of the wavelet.

The wavelets should have the following properties.

**Properties 22.** Wavelet assumptions

$P_1.$   $\{\psi_\lambda : \lambda \in \mathcal{J}\}$  is a Riesz basis for  $L_2(\mathcal{I})$ ,

$P_2.$   $\{2^{-|\lambda|t}\psi_\lambda : \lambda \in \mathcal{J}\}$  is a Riesz basis for  $W_2^t(\mathcal{I})$ ,

Denoting the dual basis of  $\{\psi_\lambda : \lambda \in \mathcal{J}\}$  for  $L_2(\mathcal{I})$  as  $\{\tilde{\psi}_\lambda : \lambda \in \mathcal{J}\}$ , furthermore we assume that for some

$$\mathbb{N} \ni d > t,$$

for all  $|\lambda| > 0$ , for some  $(\operatorname{supp} \tilde{\psi}_\lambda)^{\operatorname{int}} \subseteq \tilde{\omega}_\lambda \subseteq \mathcal{I}$ ,

$P_3.$   $|\langle \tilde{\psi}_\lambda, u \rangle_{L_2(\mathcal{I})}| \lesssim 2^{-|\lambda|d} |u|_{W_2^d(\tilde{\omega}_\lambda)}$  ( $u \in W_2^d(\mathcal{I})$ ),

$P_4.$   $\sup_{\lambda \in \mathcal{J}} 2^{|\lambda|} \max(\operatorname{diam} \tilde{\omega}_\lambda, \operatorname{diam} \operatorname{supp} \psi_\lambda) \approx \inf_{\lambda \in \mathcal{J}} 2^{|\lambda|} \max(\operatorname{diam} \tilde{\omega}_\lambda, \operatorname{diam} \operatorname{supp} \psi_\lambda)$ ,

$P_5.$   $\sup_{j, k \in \mathbb{N}_0} \#\{|\lambda| = j : [k2^{-j}, (k+1)2^{-j}] \cap (\overline{\tilde{\omega}_\lambda} \cup \operatorname{supp} \psi_\lambda) \neq \emptyset\} < \infty$ ; and  $\overline{\mathcal{I}} = \bigcup_{|\lambda|=j} \operatorname{supp} \psi_\lambda$ .

The conditions  $(P_4)$  and  $(P_5)$  will be referred to by saying that both primal and dual wavelets are *localized* or *locally finite*, respectively. Denoting the unit cube for  $n \in \mathbb{N}$  with  $\square := \mathcal{I}^n$ , the equalities  $L_2(\square) = \otimes_{i=1}^n L_2(\mathcal{I})$  and

$$W_2^t(\square) := W_2^t(\mathcal{I}) \otimes L_2(\mathcal{I}) \otimes \cdots \otimes L_2(\mathcal{I}) \cap \cdots \cap L_2(\mathcal{I}) \otimes \cdots \otimes L_2(\mathcal{I}) \otimes W_2^t(\mathcal{I}),$$

hold.

The *anisotropic tensor product wavelet* collection

$$\Psi := \{\psi_\lambda := \psi_{\lambda_1} \otimes \cdots \otimes \psi_{\lambda_n} : \lambda \in \mathcal{J} := \prod_{i=1}^n \mathcal{J}\},$$

and its renormalized version  $\{(\sum_{i=1}^n 4^{|\lambda_i|})^{-t/2} \psi_\lambda : \lambda \in \mathcal{J}\}$  are Riesz bases for  $L_2(\square)$  and  $W_2^t(\square)$ , respectively. The collection that is dual to  $\Psi$  reads as

$$\tilde{\Psi} := \{\tilde{\psi}_\lambda := \tilde{\psi}_{\lambda_1} \otimes \cdots \otimes \tilde{\psi}_{\lambda_n} : \lambda \in \mathcal{J}\}.$$

For  $\lambda \in \mathcal{J}$ , we set  $|\lambda| = (|\lambda_1|, \dots, |\lambda_n|)$ .

**Remark 23.** (i) Constructions of anisotropic tensor wavelets that satisfy essential boundary conditions also exist.

(ii) The anisotropic tensor wavelet construction differs from standard *isotropic* tensor wavelet constructions by the fact that wavelets on different levels are tensorized with each other, leading to rectangular and highly anisotropic supports.

(iii) Suitable constructions of isotropic wavelets on domains can be found, e.g., in [DS98, DS99a, DS99b, CTU00]. We also refer to [Coh00] for a detailed discussion. A generalized construction for anisotropic tensor wavelets on complex domains will be presented in a forthcoming paper.

For  $\theta \geq 0$ , the *weighted Sobolev space*  $H_\theta^d(\mathcal{I})$  is defined as the space of all measurable functions  $u$  on  $\mathcal{I}$  for which the norm

$$\|u\|_{H_\theta^d(\mathcal{I})} := \left[ \sum_{j=0}^d \int_{\mathcal{I}} |x^\theta u^{(j)}(x)|^2 dx \right]^{\frac{1}{2}}$$

is finite. For

$$m \in \{0, \dots, \lfloor t \rfloor\},$$

we will consider the weighted space

$$H_{m,\theta}^d(\square) := \cap_{p=1}^n \otimes_{i=1}^n H_{\theta - \delta_{pi} \min(m,\theta)}^d(\mathcal{I}),$$

equipped with the norm

$$\|u\|_{H_{m,\theta}^d(\square)}^2 := \sum_{i=1}^n \|u\|_{\otimes_{i=1}^n H_{\theta - \delta_{pi} \min(m,\theta)}^d(\mathcal{I})}^2.$$

It is one of the most important advantages of anisotropic tensor wavelets that they give rise to dimension-independent approximation rates, provided that the object one wants to approximate has sufficient smoothness in the weighted Sobolev scale.

**Theorem 24** ([?, Thm. 4.3]). For any  $\theta \in [0, d)$ , there exist a (nested) sequence  $(\mathcal{J}_M^{(\sigma)})_{M \in \mathbb{N}} \subset \mathcal{J}_\sigma$  with  $\#\mathcal{J}_M^{(\sigma)} \approx M$ , such that

$$\inf_{v \in \text{span}\{\psi_\lambda^{(\sigma)} : \lambda \in \mathcal{J}_M^{(\sigma)}\}} \|u - v\|_{W_2^m(\square)} \lesssim M^{-(d-m)} \|u\|_{H_{m,\theta}^d(\square)}, \quad (u \in H_{m,\theta}^d(\square) \cap W_2^m(\square)),$$

where for  $m = 0$ ,  $M^{-(d-m)}$  should be read as  $(\log \#M)^{(n-1)(\frac{1}{2}+d)} M^{-d}$ .

## 5.2 Adaptive Wavelet Schemes for Elliptic Problems

In this section, we briefly recall how wavelets can be used to treat elliptic operator equations of the form

$$\mathcal{A}u = f, \quad (25)$$

where we will assume  $\mathcal{A}$  to be a boundedly invertible operator from some Hilbert space  $\mathcal{H}$  into its normed dual  $\mathcal{H}'$ , i.e.,

$$\|\mathcal{A}u\|_{\mathcal{H}'} \sim \|u\|_{\mathcal{H}}, \quad u \in \mathcal{H}. \quad (26)$$

We shall only discuss the basic ideas, for further information, the reader is referred to [DDHS97, CDD01, CDD02]. In our application,  $\mathcal{H}$  will typically be a Sobolev space  $W_2^s(\Omega)$ . We shall mainly focus on the special case where

$$a(v, w) := \langle \mathcal{A}v, w \rangle \quad (27)$$

defines a *symmetric* bilinear form on  $\mathcal{H}$  which is *elliptic* in the sense that

$$a(v, v) \sim \|v\|_{\mathcal{H}}^2. \quad (28)$$

Usually, operator equations of the form (25) are solved by a Galerkin scheme, i.e., one defines an increasing sequence of finite dimensional approximation spaces  $S_{\Lambda_l} := \text{span}\{\eta_\mu : \mu \in \Lambda_l\}$ , where  $S_{\Lambda_l} \subset S_{\Lambda_{l+1}}$ , and projects the problem onto these spaces, i.e.,

$$\langle \mathcal{A}u_{\Lambda_l}, v \rangle = \langle f, v \rangle \quad \text{for all } v \in S_{\Lambda_l}.$$

To compute the actual Galerkin approximation, one has to solve a linear system

$$\mathbf{G}_{\Lambda_l} \mathbf{c}_{\Lambda_l} = \mathbf{f}_{\Lambda_l}, \quad \mathbf{G}_{\Lambda_l} = (\langle \mathcal{A}\eta_{\mu'}, \eta_\mu \rangle)_{\mu, \mu' \in \Lambda_l}, \quad (\mathbf{f}_{\Lambda_l})_\mu = \langle f, \eta_\mu \rangle, \quad \mu \in \Lambda_l.$$

Then the question arises how to choose the approximation spaces in a suitable way, for doing that in a somewhat clumsy fashion would yield a very inefficient scheme. One natural idea would be to use an *adaptive* scheme, i.e., an updating strategy which essentially consists of the following three steps:

solve	—	estimate	—	refine
$\mathbf{G}_{\Lambda_l} \mathbf{c}_{\Lambda_l} = \mathbf{f}_{\Lambda_l}$		$\ u - u_{\Lambda_l}\  = ?$ a posteriori error estimator		add functions if necessary.

Already the second step is highly nontrivial since the exact solution  $u$  is unknown, so that clever a posteriori error estimators are needed. Then another challenging task is to show that the refinement strategy leads to a convergent scheme and to estimate its order of convergence, if possible. In recent years, it has been shown that both tasks can be solved if wavelets are used as basis functions for the Galerkin scheme as we shall now explain.

The first step is to transform (25) into a discrete problem. By using the Riesz property ( $P_2$ ) of the wavelet basis it is easy to see that (25) is equivalent to

$$\mathbf{A}\mathbf{u} = \mathbf{f} \quad (29)$$

where

$$\mathbf{A} := \mathbf{D}^{-1} \langle \mathcal{A}\Psi, \Psi \rangle^T \mathbf{D}^{-1}, \quad \mathbf{u} := \mathbf{D}\mathbf{c}, \quad \mathbf{f} := \mathbf{D}^{-1} \langle f, \Psi \rangle^T, \quad \mathbf{D} = (2^{-s|\lambda|} \delta_{\lambda,\lambda'})_{\lambda,\lambda' \in \mathcal{J}}.$$

Now (28) implies that

$$\|\mathbf{A}\|_{\ell_2}, \|\mathbf{A}^{-1}\|_{\ell_2} < \infty,$$

and the computation of the Galerkin approximation amounts to solving the system

$$\mathbf{A}_\Lambda \mathbf{u}_\Lambda = \mathbf{f}_\Lambda := \mathbf{f}|_\Lambda, \quad \mathbf{A}_\Lambda := (2^{-s(|\lambda|+|\nu|)} \langle \psi_\lambda, \mathcal{A}\psi_\nu \rangle)_{\lambda,\nu \in \Lambda}.$$

Now, ellipticity (28) and Riesz property yield

$$\|\mathbf{u} - \mathbf{u}_\Lambda\|_{\ell_2} \sim \|\mathbf{A}(\mathbf{u} - \mathbf{u}_\Lambda)\|_{\ell_2} \sim \|\mathbf{f} - \mathbf{A}(\mathbf{u}_\Lambda)\|_{\ell_2} \sim \|\mathbf{r}_\Lambda\|_{\ell_2},$$

so that the  $\ell_2$ -norm of the *residual*  $\mathbf{r}_\Lambda$  serves as an a posteriori error estimator. Each individual coefficient  $(\mathbf{r}_\Lambda)_\lambda$  can be viewed as a local error indicator. Therefore a natural adaptive strategy would consist in catching the bulk of the residual, i.e., to choose the new index set  $\hat{\Lambda}$  such that

$$\|\mathbf{r}_\Lambda|_{\hat{\Lambda}}\|_{\ell_2} \geq \zeta \|\mathbf{r}_\Lambda\|_{\ell_2}, \quad \text{for some } \zeta \in (0, 1).$$

However, such a scheme would not be implementable since the residual involves infinitely many coefficients. To transform this idea into an implementable scheme, the following three subroutines are needed:

- **RHS** $[\varepsilon, \mathbf{g}] \rightarrow \mathbf{g}_\varepsilon$ : determines for  $\mathbf{g} \in \ell_2(\mathcal{J})$  a finitely supported  $\mathbf{g}_\varepsilon \in \ell_2(\mathcal{J})$  such that

$$\|\mathbf{g} - \mathbf{g}_\varepsilon\|_{\ell_2(\mathcal{J})} \leq \varepsilon; \quad (30)$$

- **APPLY** $[\varepsilon, \mathbf{N}, \mathbf{v}] \rightarrow \mathbf{w}_\varepsilon$ : determines for  $\mathbf{N} \in L(\ell_2(\mathcal{J}))$  and for a finitely supported  $\mathbf{v} \in \ell_2(\mathcal{J})$  a finitely supported  $\mathbf{w}_\varepsilon$  such that

$$\|\mathbf{N}\mathbf{v} - \mathbf{w}_\varepsilon\|_{\ell_2(\mathcal{J})} \leq \varepsilon; \quad (31)$$

- **COARSE** $[\varepsilon, \mathbf{v}] \rightarrow \mathbf{v}_\varepsilon$ : determines for a finitely supported  $\mathbf{v} \in \ell_2(\mathcal{J})$  a finitely supported  $\mathbf{v}_\varepsilon \in \ell_2(\mathcal{J})$  with at most  $N$  significant coefficients, such that

$$\|\mathbf{v} - \mathbf{v}_\varepsilon\|_{\ell_2(\mathcal{J})} \leq \varepsilon. \quad (32)$$

Moreover,  $N \lesssim N_{\min}$  holds,  $N_{\min}$  being the minimal number of entries for which (32) is valid.

Then, employing the key idea outlined above, the resulting fundamental algorithm reads as follows:

**ALGORITHM 25.** **SOLVE** $[\varepsilon, \mathbf{A}, \mathbf{f}] \rightarrow \mathbf{u}_\varepsilon$ :

Fix target accuracy  $\varepsilon$ ,  $\Lambda_0 := \emptyset$ ,  $\mathbf{r}_{\Lambda_0} := \mathbf{f}$ ,  $\varepsilon_0 := \|\mathbf{f}\|_{\ell_2}$ ,  $j := 0$

While  $\varepsilon_j > \varepsilon$  do

$j := j + 1$

$\varepsilon_j := 2^{-(j+1)}\|\mathbf{f}\|_{\ell_2}$ ,  $\Lambda_{j,0} := \Lambda_j$ ,  $\mathbf{u}_{j,0} := \mathbf{u}_j$ ;

  For  $k = 1, \dots, K$  do

    Compute Galerkin approximation  $\mathbf{u}_{\Lambda_{j,k-1}}$  for  $\Lambda_{j,k-1}$ ;

    Compute  $\tilde{\mathbf{r}}_{\Lambda_{j,k-1}} := \mathbf{RHS}[c_1\varepsilon_{j+1}, \mathbf{f}] - \mathbf{APPLY}[c_2\varepsilon_{j+1}, \mathbf{A}, \mathbf{u}_{\Lambda_{j,k-1}}]$ ;

    Compute smallest set  $\Lambda_{j,k}$  s.t.  $\|\tilde{\mathbf{r}}_{\Lambda_{j,k-1}}|_{\Lambda_{j,k}}\|_{\ell_2} \geq \frac{1}{2}\|\tilde{\mathbf{r}}_{\Lambda_{j,k-1}}\|_{\ell_2}$ ;

  od

**COARSE** $[c_3\varepsilon_{j+1}, \mathbf{u}_{\Lambda_{j,k}}] \rightarrow (\Lambda_{j+1}, \mathbf{u}_{j+1})$

od

**Remark 26.** (i) We shall not discuss in detail the concrete numerical realization of the three fundamental subroutines. The subroutine **COARSE** consists of a thresholding step, whereas **RHS** essentially requires the computation of a best  $n$ -term approximation. The most complicated building block is **APPLY**. Let us just mention that for elliptic operators with Schwartz kernels, the cancellation property of wavelets can be used to establish its existence. For further details, the reader is referred to [CDD01, CDD02, Ste03].

- (ii) In **ALGORITHM 25**,  $c_1, c_2$  and  $c_3$  denote some suitably chosen constants whose concrete values depend on the problem at hand. Also the parameter  $K$  has to be chosen in a suitable way. We refer again to [CDD01] for details.

It can be shown that **ALGORITHM 25** has the following basic properties:

- **ALGORITHM 25** is guaranteed to converge for a huge class of problems, i.e.

$$\|\mathbf{u} - \mathbf{u}_\varepsilon\| \lesssim \varepsilon;$$

- The order of convergence of **ALGORITHM 25** is optimal in the sense that it asymptotically realizes the convergence order of best  $n$ -term wavelet approximation, i.e., if the best  $n$ -term approximation satisfies  $\mathcal{O}(n^{-s})$ , then

$$\|\mathbf{u} - \mathbf{u}_\varepsilon\| = \mathcal{O}((\#\text{supp}\mathbf{u}_\varepsilon)^{-s});$$

- The number of arithmetic operations stays proportional to the number of unknowns, that is, the number of flops needed to compute  $\mathbf{u}_\varepsilon$  satisfies  $\mathcal{O}(\#\text{supp}\mathbf{u}_\varepsilon)$ .

**Remark 27.** The analysis in this chapter was treated for the linear case. Generalizations to the nonlinear case exist by now, see [CDD03, Bar05, DSX00, Kap]. However, the theory is only fully established for the isotropic case. For first results concerning the anisotropic case we refer to [SS09]. These specific results are based on interpolets.

### 5.3 Adaptive Wavelet Schemes for Parabolic Problems

In this section, we turn to the development of adaptive wavelet-based numerical schemes for linear parabolic problems of the form (11). We assume that we are given a Gelfand triple  $V \hookrightarrow G \hookrightarrow V'$  of Hilbert spaces and that  $\mathcal{A}(t) : V \rightarrow V'$  fits into the setting of Section 5.2. Moreover, we assume that  $-\mathcal{A}(t) : D(\mathcal{A}) \subset G \rightarrow G$  is *sectorial*, i.e., there are constants  $z_0 \in \mathbb{R}$ ,  $\omega_0 \in (\frac{\pi}{2}, \pi)$  and  $M > 0$ , such that the resolvent set  $\rho(-\mathcal{A}(t))$  contains the open sector

$$\Sigma_{z_0, \omega_0} := \{z \in \mathbb{C} \setminus \{z_0\} : |\arg(z - z_0)| < \omega_0\}, \quad (33)$$

and the resolvent operator  $R(\lambda, -\mathcal{A}(t)) := (\lambda I + \mathcal{A}(t))^{-1}$  of  $-\mathcal{A}(t)$  is bounded in norm by

$$\|R(z, -\mathcal{A}(t))\|_{\mathcal{L}(X)} \leq \frac{M}{|z - z_0|}, \quad z \in \Sigma_{z_0, \omega_0}. \quad (34)$$

We may then consider (11) as an abstract initial value problem for a Hilbert space-valued variable  $u : [0, T] \rightarrow V$ . For its numerical treatment, we use the Rothe method which is also known as the horizontal method of lines. Doing so, the discretisation is performed in two major steps. Firstly, we consider a semidiscretisation in time, where we will employ an  $S$ -stage linearly implicit scheme. We shall end up with an orbit of approximations  $u^{(n)} \in L_2(\Omega)$  at intermediate times  $t_n$  that are implicitly given via the  $S$  elliptic stage equations. In a finite element context, this very approach has already been propagated in [Lan99, Lan01]. For the realization of the increment  $u^{(n)} \mapsto u^{(n+1)}$  and the spatial discretisation of the stage equations, we will then employ the adaptive wavelet scheme introduced in Section 5.2 as a black box solver.

Let us start with the time discretisation. In order to obtain a convenient notation, we will consider (11) in the generalized form

$$u'(t) = H(t, u(t)), \quad t \in (0, T], \quad u(0) = u_0, \quad (35)$$

where  $H : [0, T] \times X \rightarrow X'$  is given as

$$H(t, v) = -\mathcal{A}(t)v + F(t, v), \quad t \in [0, T], \quad v \in G. \quad (36)$$

We consider an  $S$ -stage linearly implicit method for the semidiscretisation in time. By this we mean an iteration of the form

$$u^{(n+1)} = u^{(n)} + h \sum_{i=1}^S b_i k_i \quad (37)$$

with the *stage equations*

$$(I - h\gamma_{i,i}J)k_i = G\left(t_n + \alpha_i h, u^{(n)} + h \sum_{j=1}^{i-1} \alpha_{i,j} k_j\right) + hJ \sum_{j=1}^{i-1} \gamma_{i,j} k_j + h\gamma_i g, \quad i = 1, \dots, S, \quad (38)$$

where we set

$$\alpha_i := \sum_{j=1}^{i-1} \alpha_{i,j}, \quad \gamma_i := \sum_{j=1}^i \gamma_{i,j}. \quad (39)$$

The operator  $I - h\gamma_{i,i}J$  in (38) has to be understood as a boundedly invertible operator from  $X$  to  $X'$ , with the equality (38) in the sense of  $X'$ . Such a scheme is also known as a method of *Rosenbrock* type, see [HW96, SW92] for details. All the quantities  $h$ ,  $J$ ,  $k_i$  and  $g$  in (38) do of course depend on the time step number  $n$ , but we drop the index  $n$  here for readability. The coefficients  $b_i$ ,  $\alpha_{i,j}$  and  $\gamma_{i,j}$  have to be suitably chosen according to the desired properties of the Rosenbrock method. As a special case of (38), a *Rosenbrock–Wanner method* or *ROW-method* results if one chooses the exact derivatives  $J = \partial_v H(t_n, u^{(n)})$  and  $g = \partial_t H(t_n, u^{(n)})$ . In this paper, we will confine the setting to these ROW-type methods.

In practice, a Rosenbrock scheme will be implemented in a slightly different way than given by (38). Introducing the variable  $u_i := h \sum_{j=1}^i \gamma_{i,j} k_j$ , the additional application of the operator  $J$  in the right-hand side of (38) can be avoided by rewriting (38) as

$$\left(\frac{1}{h\gamma_{i,i}}I - J\right)u_i = H\left(t_n + \alpha_i h, u^{(n)} + \sum_{j=1}^{i-1} a_{i,j} u_j\right) + \sum_{j=1}^{i-1} \frac{c_{i,j}}{h} u_j + h\gamma_i g, \quad i = 1, \dots, S, \quad (40)$$

and

$$u^{(n+1)} = u^{(n)} + \sum_{i=1}^S m_i u_i \quad (41)$$

where we have used the coefficients

$$\Gamma = (\gamma_{i,j})_{i,j=1}^S, \quad (42)$$

$$(a_{i,j})_{i,j=1}^S = (\alpha_{i,j})_{i,j=1}^S \Gamma^{-1}, \quad (43)$$

$$(c_{i,j})_{i,j=1}^S = \text{diag}(\gamma_{1,1}^{-1}, \dots, \gamma_{S,S}^{-1}) - \Gamma^{-1}, \quad (44)$$

$$(m_1, \dots, m_S)^\top = (b_1, \dots, b_S)^\top \Gamma^{-1}. \quad (45)$$

It is well-known that for a strongly  $A(\theta)$ -stable Rosenbrock method the numerical approximations according to (37) indeed converge to the exact solution as  $h \rightarrow 0$ , see

[LO95] for details. However, a constant temporal step size  $h$  might not be the most economic choice. At least for times  $t$  close to 0 and in situations where the driving term  $f$  is not smooth at  $t$ , it is advisable to choose small values of  $h$  in order to track the behaviour of the exact solution correctly. In regions where  $f$  and  $u$  are temporally smooth, larger time step sizes may be used. As a consequence, we have to employ an a posteriori temporal error estimator to control the current value of  $h$ . The traditional approach resorts to estimators for the local truncation error at  $t_n$

$$\delta_h(t_n) := \Phi^{t_n, t_n+h}(u(t_n)) - u(t_n + h), \quad (46)$$

where  $\Phi^{t_n, t_n+h} : V \rightarrow V$  is the increment mapping of the given Rosenbrock scheme at time  $t_n$  with step size  $h$ . For the global error at  $t = t_{n+1} = t_n + h_n$ , we have the decomposition

$$e_{n+1} = u^{(n+1)} - u(t_{n+1}) = \Phi^{t_n, t_n+h_n}(u^{(n)}) - \Phi^{t_n, t_n+h_n}(u(t_n)) + \delta_{h_n}(t_n), \quad (47)$$

i.e.,  $e_{n+1}$  comprises the local error at time  $t_n$  and the difference between the current Rosenbrock step  $\Phi^{t_n, t_n+h_n}(u^{(n)})$  and the virtual step  $\Phi^{t_n, t_n+h_n}(u(t_n))$  with starting point  $u(t_n)$ . Estimators for the local discretisation error  $\delta_{h_n}(t_n)$  can be either based on an embedded lower order scheme or on extrapolation techniques, see [HNW93, HW96]. For applications to partial differential equations, embedding strategies yield sufficient results and thus are our method of choice.

Since the iteration (37) cannot be implemented numerically, we will now finally address the numerical approximation of all the ingredients by finite-dimensional counterparts. Precisely, we have to find approximate, computable iterands  $\tilde{u}^{(n+1)}$ , such that the additional error  $\tilde{u}^{(n+1)} - u^{(n+1)}$  introduced by the spatial discretisation stays below some given tolerance  $\varepsilon$  when measured in an appropriate norm. Hence this perturbation of the virtual orbit  $\{u^{(n)}\}_{n \geq 0}$  can be interpreted as a controllable additional error of the temporal discretisation. The accumulation of local perturbations in the course of the iteration is then an issue for the step size controller. In order not to spoil the convergence behaviour of the unperturbed iterands  $u^{(n)}$  we will demand that  $\tilde{u}^{(n+1)} - u^{(n+1)}$  stays small in the topology of  $V$ , which results in the requirement

$$\|\tilde{u}^{(n+1)} - u^{(n+1)}\|_V \leq \varepsilon \quad (48)$$

for the numerical scheme, where  $\varepsilon > 0$  is the desired target accuracy. To achieve this goal, we want to use the convergent adaptive wavelet schemes as outlined in Subsection 5.2. Observe that by (41), the exact increment  $u^{(n+1)}$  differs from  $u^{(n)}$  by a linear combination of the exact solutions  $u_i$  of the  $S$  stage equations (40).

In case that the ellipticity constants of  $-\mathcal{A}(t)$  do not depend on  $t$  and we choose  $J = -\mathcal{A}(t)$ , the operators involved in (40) take the form

$$B_\alpha := \alpha I + \mathcal{A}(t), \quad \alpha \geq 0, \quad (49)$$

where  $\alpha = (h\gamma_{i,i})^{-1}$  for the  $i$ -th stage equation. By the estimate

$$\langle B_0 v, v \rangle \leq \langle B_\alpha v, v \rangle = \alpha \langle v, v \rangle_V + \langle B_0 v, v \rangle \leq (C\alpha + 1) \langle B_0 v, v \rangle, \quad v \in V,$$

we see that the energy norms  $\|v\|_{B_\alpha} := |\langle B_\alpha v, v \rangle|^{1/2}$  differ from  $\|v\|_{B_0} \approx \|v\|_V$  only by an  $\alpha$ -dependent constant:

$$\|v\|_{B_0} \leq \|v\|_{B_\alpha} \leq (C\alpha + 1)^{1/2} \|v\|_{B_0}, \quad v \in V. \quad (50)$$

Consequently, if we define

$$(\mathbf{D}_\alpha)_{\lambda,\lambda} := \|\psi_\lambda\|_{B_\alpha}, \quad \lambda \in \mathcal{J}, \quad (51)$$

then the system  $\mathbf{D}_\alpha^{-1}\Psi$  is a Riesz basis in the energy space  $(V, \|\cdot\|_{B_\alpha})$ , with Riesz constants independent from  $\alpha \geq 0$ :

$$\|\mathbf{c}\|_{\ell_2} \sim \|\mathbf{c}^\top \mathbf{D}_\alpha^{-1} \Psi\|_{B_\alpha}, \quad \mathbf{c} \in \ell_2. \quad (52)$$

Therefore, we can use the Riesz basis  $\mathbf{D}_\alpha^{-1}\Psi$ ,  $\alpha = (h\gamma_{i,i})^{-1}$  as test functions in a variational formulation of (40). Abbreviating the exact right-hand side of (40) by

$$r_{i,h} := H\left(t_n + \alpha_i h, u^{(n)} + \sum_{j=1}^{i-1} a_{i,j} u_j\right) + \sum_{j=1}^{i-1} \frac{c_{i,j}}{h} u_j + h\gamma_i g, \quad (53)$$

we get the system of equations

$$\langle B_\alpha u_i, \mathbf{D}_\alpha^{-1} \Psi \rangle^\top = \langle r_{i,h}, \mathbf{D}_\alpha^{-1} \Psi \rangle^\top. \quad (54)$$

Inserting a wavelet representation of  $u_i = (\mathbf{D}_\alpha \mathbf{u}_i)^\top \mathbf{D}_\alpha^{-1} \Psi$  into the variational formulation (54), we end up with the biinfinite linear system in  $\ell_2$

$$\mathbf{D}_\alpha^{-1} \langle B_\alpha \Psi, \Psi \rangle^\top \mathbf{D}_\alpha^{-1} \mathbf{D}_\alpha \mathbf{u}_i = \mathbf{D}_\alpha^{-1} \langle r_{i,h}, \Psi \rangle^\top. \quad (55)$$

Now we observe that problem (55) exactly fits into the setting of Subsection 5.2.

A detailed analysis of the concepts outlined above can be found in the PhD thesis [Raa07].

## 6 Numerical experiments

In this section we want to apply the algorithms outlined in Section 4 and 5 to identify the unknown parameters in the fundamental problem (1) from given data.

As a first step and as a proof of concept, we consider a linearized version of (1). As outlined in Remark 27, this is required in order to justify the adaptive wavelet solver. Moreover we restrict ourselves to the scalar valued case  $N = 1$ , i.e. this refers to the simple model for the concentration of a single gene, and we concentrate on the identification of the interaction matrix  $W$ , see again Subsection 2.1 for details, which still poses a non-linear inverse problem.

In order to apply sparsity concepts we need to specify the function system for which we assume a sparse representation of the searched for parameter. We choose the most convenient wavelet basis for our proof of principle, i.e. we assume the  $W$  has a sparse Haar wavelet representation.

## 6.1 An Algorithm for a Model Problem

We consider the case of a single gene, that is  $N = 1$ , i.e.  $W$  is a scalar valued function. For the reasons outlined above we restrict ourselves to a linearized version of the model equation where the sigmoidal is replaced by  $\Phi(x) = 1/2(x+1)$ . For simplicity we choose  $T = 1$  and set  $D = 1, \lambda = 0, R = 1$  and want to identify  $W \in L_2(0, 1, L_2(U, \mathbb{R}^n))$ , where  $U \subset \mathbb{R}^n, n \in \{1, 2\}$ . As the penalty term in (20) we use the weighted  $\ell_1$ -norm of the wavelet coefficients with respect to the Haar basis. The noise level is 0 in these first experiments. The regularization parameters are therefore handpicked and do not follow any parameter choice rule.

In this setting the control-to-state operator  $\mathfrak{D}$  maps the parameter  $W$  to the solution  $u$  of the parabolic model problem

$$u' - \Delta u - Wu = \frac{1}{2}, \quad u(0) = u_0, \quad \frac{\partial u}{\partial \nu} \Big|_{\partial U \times (0,1)} = 0. \quad (56)$$

The given data corresponding to the looked for parameter will be denoted by  $y_{data} = \mathfrak{D}(W)$ .

The remaining task is to identify the solution of the adjoint problem that has to be solved at each iteration of (23). It is given by  $(\mathfrak{D}'(p))^*(w)$ , with  $w = \mathfrak{D}(p) - y_{data}$  and can be solved using the explicit formulas given in Remark 19:

$$-h' - \Delta h - Wh = w, \quad h(1) = 0, \quad \frac{\partial h}{\partial \nu} \Big|_{\partial U \times (0,1)} = 0. \quad (57)$$

All parabolic problems are solved with the Rothe method, see Section 5.3, using inexact linearly implicit increments [Raa07]. For the experiments, we choose the second-order Rosenbrock scheme ROS2. The elliptic subproblems are discretized by means of an anisotropic tensor wavelet basis for  $W_2^1(U)$ , see Section 5.1. They are solved with the adaptive wavelet-Galerkin algorithm **ALGORITHM 25**. The discretization of the operator  $\mathcal{A}^{(n)}(t) = -\Delta + W^{(n)}(t) \text{Id}$  in the  $n$ -th iteration step at time  $t$  is denoted with  $\mathbf{A}^{(n)}(t)$ . The parameter space  $L_2(U)$  is discretized by means of an isotropic Haar wavelet basis. As a slight abuse of notation we denote all wavelet coefficient vectors with boldface letters and drop the dependence on  $t$  in the following algorithm.

Inserting the Equations (56) and (57) into the fixpoint iteration determined by (23) the algorithm for solving the parameter identification problem reads as follows.

1.  $n = 0$ ,  $\mathbf{W}^{(0)} = 0$ . Initialize the Haar wavelet coefficients  $\mathbf{W}^{(0)}$  and anisotropic tensor wavelet coefficients  $\mathbf{u}_0$ .
2. Compute the solution  $\mathbf{u}^{(n)}$  of (56) with parameter  $\mathbf{W}^{(n)}$ .
3. Compute the solution  $\mathbf{h}^{(n)}$  of (57) with the right-hand side given by  $\mathbf{w} = \mathbf{u}^{(n)} - \mathbf{Y}_{data}$ .
4. Compute the Haar wavelet coefficients of the product  $u^{(n)} \cdot h^{(n)}$ . Denoted the result by  $\mathbf{u}^{(n)} \cdot \mathbf{h}^{(n)}$ .

5. Apply shrinkage and compute  $\mathbf{W}^{(n+1)} = S_\alpha(\mathbf{W}^{(n)} - \mathbf{u}^{(n)} \cdot \mathbf{h}^{(n)})$ , where  $S_\alpha$  is given by (24).
6. Check stopping criterion  $\|\mathbf{W}^{(n+1)} - \mathbf{W}^{(n)}\|_{\ell_2} / \|\mathbf{W}^{(n)}\|_{\ell_2} \leq tol$ . If needed increase  $n$  and go to 2.

Since all computed coefficient vectors are finite it is possible to realize the product in step 4 by computing Haar generator coefficients of  $u^{(n)}$  and  $h^{(n)}$  on a sufficiently high level and multiply those coefficients.  $S_\alpha$  is applied at each time step and to each coefficient. For the sake of comparability of the results we also introduced a maximum iteration number. The attentive reader notices that we did not perform the step size control after the shrinkage step, in order to simplify the implementation. Convergence nonetheless is ensured (compare also [BLM09, p. 187]).

For completeness we note that the Haar wavelet basis in one dimension is given by  $\{1_{(0,1)}\} \cup \{\psi_{j,k} : j \in \mathbb{N}_0, 1 \leq k \leq 2^j\}$ , with  $\psi_{j,k}(x) = 2^{j/2}\psi(2^jx - k)$ , where

$$\psi(x) = \begin{cases} 1 & x \in (0, \frac{1}{2}], \\ -1 & x \in (\frac{1}{2}, 1), \\ 0 & \text{otherwise.} \end{cases}$$

## 6.2 Experiments in one spatial dimension

For the case  $n = 1$  we considered the interval  $U = (0, 1)$ . Biorthogonal wavelets, as designed in [Pri06], were used as a basis for  $H^1(U)$ . We used wavelets with primal and dual order  $d = \tilde{d} = 3$ , fulfilling Properties 22. In order to realize a high amount of iterations in reasonable time we limited our computation to an equidistant time discretization with 10 time steps and introduced a maximum level of wavelets considered for the biorthogonal basis of  $j = 6$  and for the Haar basis of 5.

For the parameters  $W \in L_2((0, 1), L_2(U))$  of (1), we assume sparsity in time and space. Therefore we choose  $W(t, x) = 1_{[0.3, 0.7]}(t) \times g(x)$ , with  $g(x) = c_0 1_{(0,1)}(x) + \sum_{j=0}^{\infty} \sum_{k=0}^{2^j} c_{j,k} \psi_{j,k}(x)$ , with three non-zero coefficients  $c_0 = c_{0,0} = 0.5$  and  $c_{1,2} = 2^{-1/2}$ , see Figure 1.

The regularization parameter  $\alpha$  was chosen as  $1e - 6, 1e - 5, 1e - 4, 1e - 3$ . In Figure 3 (left image) the discrepancy  $\|\mathbf{u}^n - \mathbf{y}_{\text{data}}\|_{\ell_2}$  is plotted versus the  $\ell_1$ -norm  $\sum_{i=1}^N 1/N \|\mathbf{w}^n(i)\|_{\ell_1}$ . This graph shows the expected monotone decrease of the error and the typical overshoot of the  $\ell_1$ -norm during the first operations of the iteration process. Note, that the iterations tends to strongly decrease the  $\ell_1$ -norm during hte final iterations at the expense of a slightly increasing residual error. The right graph plots the error versus the iteration number.

Overall, as to be expected from a standard gradient type method, the convergence is rather slow. The residual error of the limit solution after 15000 iterations as well as the convergence behaviour are presented in Figure 6.2.

At a first glance and taking into account, that the true solution has only three non-zero coefficients and the noise level has been set to 0, it seems to be counter intuitive, that

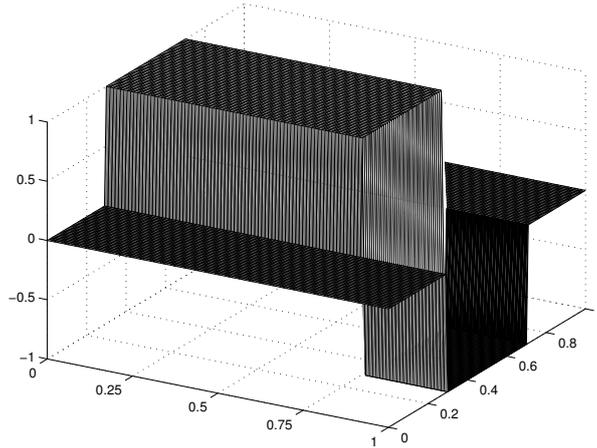


Figure 1: Exact parameter  $W$  for the 1 dimensional case.

the reconstructions exhibit a rather larger number of non-zero coefficients. This is due to the interplay between the discretization of the parameter  $W$  and the wavelet basis for representation the solution  $u$  of the parabolic equation. For  $u$  a piecewise linear wavelet basis was chosen. However, this needs to be converted to a Haar-Wavelet expansion in Step 4 of the algorithm in order to perform the product  $h \cdot u$  as well as the shrinkage operation in Step 5. Similarly, the sparse Haar wavelet expansion for  $W$  results in a non-sparse expansion in terms of piecewise linear wavelets in Step 2 of the algorithm. Overall, this leads to a smoothed reconstruction of  $W$ , which is less sparse than the true solution.

### 6.3 Experiments in 2 dimensions

For the two dimensional case we consider the unit cube  $U = (0, 1)^2$ . The spatial discretization consists of biorthogonal anisotropic tensor wavelets as described in Section 5.1. We use the same 1 dimensional bases for the construction as in the previous section.

For this example we consider a fixed time discretization with 6 time steps, and maximum levels of 6 and 4 for the anisotropic tensor wavelet basis and Haar basis, respectively.

Following the chain of thought of the 1 dimensional case we try to reconstruct a single generator at different time steps and define  $W = 1_{[1/3, 2/3]} \times 1_{[0.5, 0.75]^2}$ , resulting in 7 active Haar coefficients.

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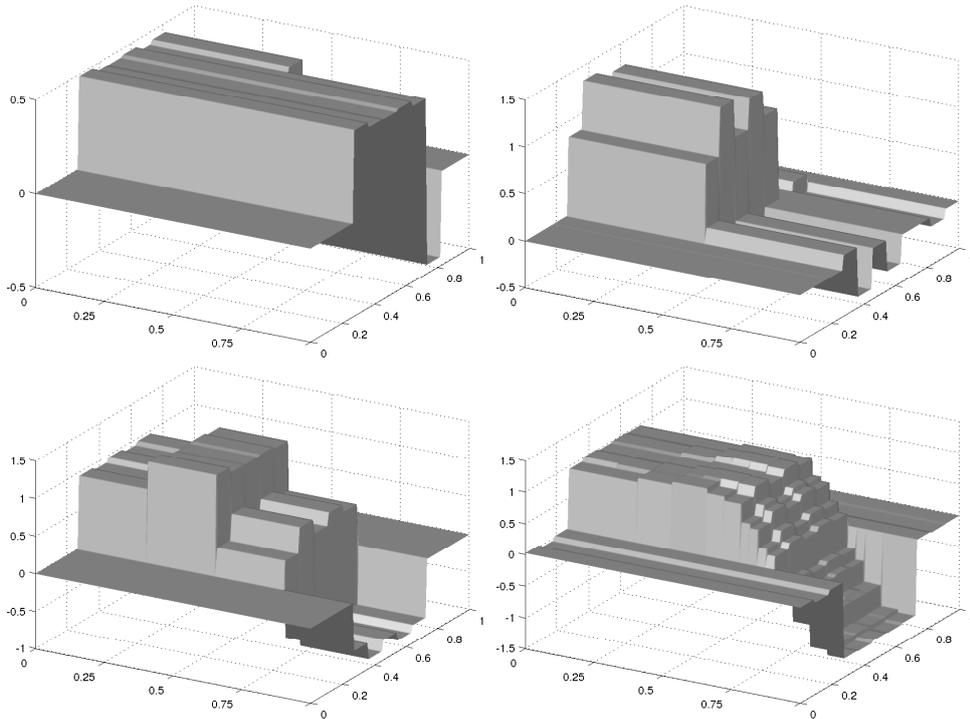


Figure 2: Reconstruction 1 dimensional case.  $\alpha = 1e - 3, 1e - 4, 1e - 5, 1e - 6$

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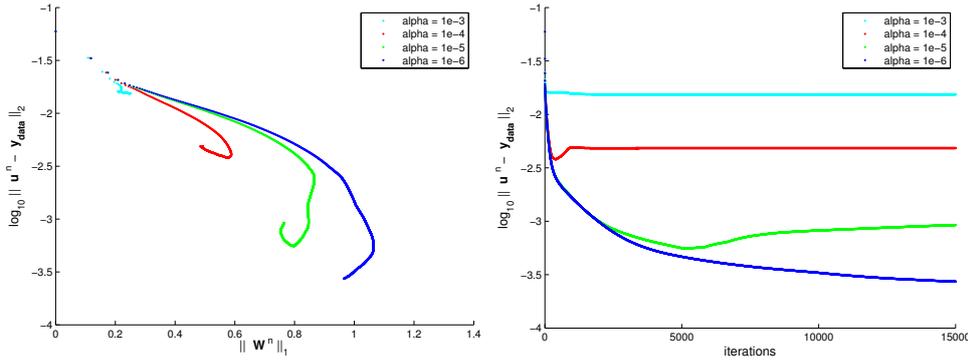


Figure 3:  $\|\mathbf{u}^* - \mathbf{y}_{\text{data}}\|_{\ell_2}$  vs  $\|\mathbf{W}^n\|_{\ell_1}$  (left) and iterations (right), 1 dimensional case.

$\alpha$	$\ \mathbf{u}^* - \mathbf{y}_{\text{data}}\ _{\ell_2}$	$\ \mathbf{W}^*\ _{\ell_1}$
1e-6	2.73e-4	0.965
1e-5	9.23e-4	0.765
1e-4	4.80e-3	0.492
1e-3	1.54e-2	0.250

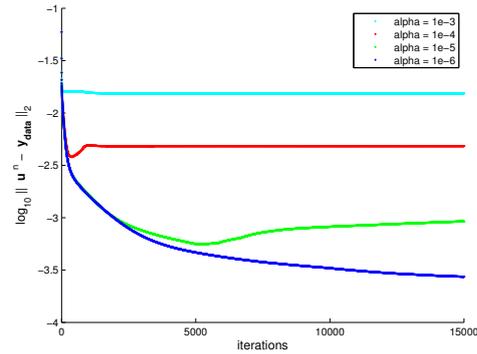


Figure 4: Left: residuum and reconstruction for certain  $\alpha$ , right: residuum vs iterations, 1 dimensional case.

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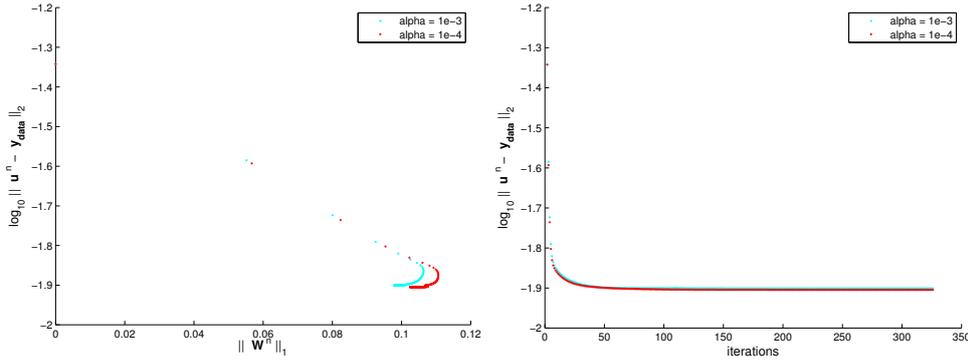


Figure 5:  $\|\mathbf{u}^* - \mathbf{y}_{\text{data}}\|_{\ell_2}$  vs  $\|\mathbf{W}^n\|_{\ell_1}$  (left), iterations (right), 2 dimensional case.

$\alpha$	$\ \mathbf{u}^* - \mathbf{y}_{\text{data}}\ _{\ell_2}$	$\ \mathbf{W}^*\ _{\ell_1}$
1e-4	1,25e-1	0.1025
1e-3	1,25e-1	0.0975

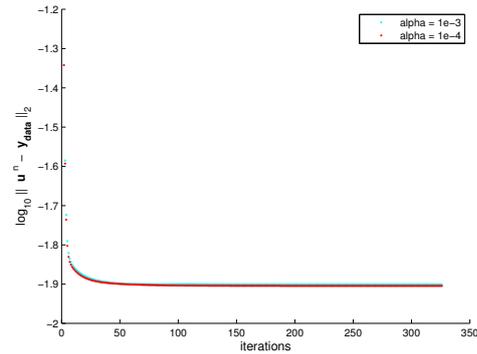


Figure 6: Left: residuum and reconstruction for certain  $\alpha$ , right: residuum vs iterations, 2 dimensional case.

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